

MATERIAL SAFETY DATA SHEET

1. SUBSTANCE AND SOURCE IDENTIFICATION

National Institute of Standards and Technology
Standard Reference Materials Program
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SRM Number: 1051b
MSDS Number: 1051b
SRM Name: Barium Cyclohexanebutyrate

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Description: This Standard Reference Material (SRM) is primarily intended for use in preparing standard oil solutions containing barium. It is essentially free from other metals and has suitable solubility, compatibility, and uniformity for use with most lubricating oils or petroleum products. Each unit consists of 5 g, with a certified barium content.

Substance: Barium Cyclohexanebutyrate

Other Designations: Barium cyclohexanebutyrate (1:2); barium salt; 4-cyclohexanebutyric acid, cyclohexanebutanoic acid.

2. COMPOSITION AND INFORMATION ON HAZARDOUS INGREDIENTS

Component:	Barium Cyclohexanebutyrate
CAS Number:	62669-65-2
EC Number (EINECS):	263-685-7
Nominal Mass Fraction (%):	29
EC Classification:	Xi (Irritant); not classified in Annex I of Directive 67/548EEC
EC Risk:	R22 (harmful if swallowed) R36/37/38 (irritating to eyes, respiratory system, and skin)
EC Safety:	S24/25 (avoid contact with skin and eyes) S45 (in case of accident or illness, see doctor; show label)

3. HAZARDS IDENTIFICATION

NFPA Ratings (Scale 0-4): Health = 1 Fire = 0 Reactivity = 0

Major Health Hazards: This barium compound can irritate the respiratory tract, skin, and eyes. Its toxicological properties have not yet been fully investigated, but its toxicity is expected to be relatively low because of its low solubility in water.

Physical Hazards: Dust-air mixture may explode. Container may shatter.

Potential Health Effects

Inhalation: Inhalation of this barium compound in powder form can irritate the respiratory tract. Barium metal fumes can cause metal fume fever, with flu-like symptoms and a metallic taste in the mouth.

Skin Contact:	Contact with this material can cause skin irritation.
Eye Contact:	This material can cause eye irritation, with possible damage to the cornea.
Ingestion:	This material can irritate the GI tract, causing abdominal pain, vomiting, and diarrhea. Its toxicity is expected to be lower than that of water-soluble barium salts. Some barium compounds can reduce serum potassium levels, causing muscular tremors and contraction, weakness, irregular heartbeat, convulsions, and paralysis. Chronic ingestion of barium may cause electrolyte imbalance and kidney damage.

Medical Conditions Aggravated by Exposure: Pre-existing conditions affecting the lungs, skin, kidneys, or other target organs.

Listed as a Carcinogen/ Potential Carcinogen:

	Yes	No
In the National Toxicology Program (NTP) Report on Carcinogens	_____	<u> X </u>
In the International Agency for Research on Cancer (IARC) Monographs	_____	<u> X </u>
By the Occupational Safety and Health Administration (OSHA)	_____	<u> X </u>

4. FIRST AID MEASURES

Inhalation: Move the person to fresh air immediately. If not breathing, qualified medical personnel may start CPR or give oxygen if necessary. Get medical aid at once, and bring the container or label.

Skin Contact: Remove contaminated clothing and shoes. Flush affected skin with water for at least 15 minutes, then wash thoroughly with soap and water. If skin irritation persists, get medical aid and bring the container or label. Wash contaminated clothing before reusing.

Eye Contact: Remove contact lenses (if any). Do not allow victim to rub eyes or keep eyes closed. Flush eyes with large amounts of running water for at least 30 minutes, keeping eyelids open and raising lids to remove all chemical. Get medical aid at once, and bring the container or label.

Ingestion: Contact a poison control center immediately for instructions. Wash out mouth with water, but do not induce vomiting. Get medical aid at once, and bring the container or label.

5. FIRE FIGHTING MEASURES

Fire and Explosion Hazards: This material is not believed to be a significant fire or explosion hazard, but dust-air mixtures may ignite or explode. See also Section 10, Incompatible Materials.

Extinguishing Media: Use extinguishing media appropriate to the surrounding fire: water spray, dry chemical, carbon dioxide, or foam. Use a water spray to cool containers.

Fire Fighting: Avoid inhalation of material or combustion byproducts. Wear full protective clothing and NIOSH-approved self-contained breathing apparatus (SCBA).

Flash Point (°C): N/A

Autoignition (°C): N/A

Lower Explosive Limit (LEL): N/A

Upper Explosive Limit (UEL): N/A

Flammability Class (OSHA): N/A

6. ACCIDENTAL RELEASE MEASURES

Occupational Release: Isolate the spill area and remove any sources of ignition. Cleanup personnel must wear personal protective equipment (Section 8). Sweep up material and place in a suitable container for reclamation or disposal, using a method that does not generate dust.

Disposal: Refer to Section 13, Disposal Considerations.

7. HANDLING AND STORAGE

Storage: Store this material in the original container at room temperature. Protect from moisture, heat, and physical damage, and isolate from incompatible materials.

Safe Handling Precautions: Wear a dust mask or respirator. Avoid contact or wash after handling.

8. EXPOSURE CONTROLS AND PERSONAL PROTECTION

Exposure Limits (Barium):

ACGIH TLV-TWA: 0.5 mg/m³

OSHA TLV-TWA: 0.5 mg/m³

UK WEL: 0.5 mg/m³

Ventilation: Use local or general exhaust to keep employee exposures below limits. Local exhaust ventilation is preferred because it can control contaminant emissions at the source, preventing dispersion into the general work area. Refer to the ACGIH document *Industrial Ventilation, a Manual of Recommended Practices*.

Respirator: If necessary, refer to the NIOSH document *Guide to the Selection and Use of Particulate Respirators Certified under 42 CFR 84* for selection and use of respirators certified by NIOSH.

Eye Protection: Use chemical safety goggles where dusting or splashing of solutions may occur. See OSHA standard (29 CFR 1910.133) or European Standard EN166. The employer should provide an emergency eye wash fountain and safety shower in the immediate work area.

Personal Protection: Wear appropriate gloves and protective clothing to prevent contact with skin.

9. PHYSICAL AND CHEMICAL PROPERTIES

Component: Barium Cyclohexanecarboxylate

Appearance and Odor: White powder, odorless

Relative Molecular Weight: 475.8

Molecular Formula: (C₆H₁₁CH₂CH₂CH₂COO)₂Ba

Density (g/cm³): N/A

Solvent Solubility: N/A

Water Solubility: Negligible

Boiling Point (°C): N/A

Melting Point (°C): N/A

Vapor Pressure (Pa): N/A

Vapor Density (Air = 1): 16.4

10. STABILITY AND REACTIVITY

Stability: X Stable Unstable

Stable at normal temperature and pressure.

Conditions to Avoid: Dust generation; incompatible materials.

Incompatible Materials: Strong oxidizers.

Fire/Explosion Information: See Section 5.

Hazardous Decomposition: Thermal decomposition of this material may produce carbon oxides (CO, CO₂).

Hazardous Polymerization: Will Occur X Will Not Occur

11. TOXICOLOGICAL INFORMATION

Route of Entry: X Inhalation X Skin X Ingestion

Toxicity Data: No toxicity data are available for this compound. Data for barium:

Rat, oral: TD_{Lo} (69 wks) = 26,622 mg/kg

Target Organ(s): Respiratory tract, skin, eyes, GI tract, kidneys.

Mutagen/Teratogen: The toxicity of this material has not been fully investigated. Some barium compounds have shown mutagenic activity in standard tests.

Health Effects: See Section 3.

12. ECOLOGICAL INFORMATION

Ecotoxicity Data (Barium):

Brown shrimp (*Penaeus aztecus*): BCF (bioconcentration factor) = 0.0020 µg/L

Sheepshead minnow (*Cyprinodon variegatus*): LC₅₀ (24 hrs) = 500,000 µg/L

Water flea (*Daphnia magna*): LC₅₀ (48 hrs) = 410,000 µg/L

Environmental Summary: This material may be slightly toxic to aquatic life, but its low solubility in water may limit its impact. Barium may bioaccumulate.

13. DISPOSAL CONSIDERATIONS

Waste Disposal: Dispose of container and unused contents in accordance with federal, state, and local requirements, which vary according to location. Although this material is not a listed RCRA hazardous waste, it may exhibit one or more characteristics of a hazardous waste and thus requires appropriate analysis to determine specific disposal requirements. Processing, use, or contamination of this product may change the waste management options.

14. TRANSPORTATION INFORMATION

U.S. DOT and IATA (Barium Compound, n.o.s.): Not regulated.

15. REGULATORY INFORMATION

U.S. REGULATIONS

CERCLA Sections 102a/103 (40 CFR 302.4): Not regulated

SARA Title III Section 302: Not regulated

SARA Title III Section 304: Not regulated

SARA Title III Section 313: Regulated (as N040, Barium Compounds)

OSHA Process Safety (29 CFR 1910.119): Not regulated

SARA Title III Sections 311/312 Hazardous Categories (40 CFR 370.21):

ACUTE:	Yes
CHRONIC:	Yes
FIRE:	No
REACTIVE:	No
SUDDEN RELEASE:	No

STATE REGULATIONS

California Proposition 65: Not regulated

CANADIAN REGULATIONS

WHMIS Classification: D2B (toxic)

WHMIS Ingredient Disclosure List: Not regulated (water-soluble barium compounds only)

CEPA Domestic Substances List (DSL): Regulated

EUROPEAN REGULATIONS

EU/EC Classification: Xi (Irritant); not classified in Annex I of Directive 67/548EEC

NATIONAL INVENTORY STATUS

U.S. Inventory (TSCA): Listed

TSCA 12(b), Export Notification: Not listed

16. OTHER INFORMATION

Sources:

Amdur M.O., et al., *Casarett and Doull's Toxicology: The Basic Science of Poisons*. 4th Ed. New York: McGraw-Hill, 1993.

PAN Pesticide Database: Barium.

U.S. National Institute for Occupational Safety and Health, *NIOSH Pocket Guide to Chemical Hazards*, September 2005 edition. DHHS (NIOSH) Publication No. 2005-151.

Disclaimer: Physical and chemical data contained in this MSDS are provided only for use as a guide in assessing the hazardous nature of the material. The MSDS was prepared carefully, using current references; however, NIST does not certify the data in the MSDS. The certified values for this material are given in the NIST Certificate of Analysis.